

Defining statistical ensembles of random graphs^{*}

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Abstract

The problem of defining a statistical ensemble of random graphs with an arbitrary connectivity distribution is discussed. Introducing such an ensemble is a step towards understanding the geometry of wide classes of graphs independently of any specific model. This research was triggered by the recent interest in the so-called scale-free networks.

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1 Introduction

This is a workshop talk and therefore I do not hesitate to report about partial results of a research still in progress. I shall also submit you a couple of queries, with the hope of attracting your interest and triggering a discussion. I have benefited from collaboration with Z. Burda, the late J.D. Correia and J. Jurkiewicz (cf ref. [1] and papers quoted therein).

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Let me recall that a graph is just a collection of vertices (nodes) and links (edges) connecting vertices. It is a mathematical idealization representing various networks one encounters in nature, in social life, in engineering, etc. For example, the web can be represented by a graph: the vertices are the URLs and the links are the hyperlinks. Likewise, the network of sexual relations in a population can be represented by a graph. The study of its geometry has some interest for epidemiology. In these examples, as in many other ones, the pattern of connections between vertices is fairly random. The concept of a *random graph* emerges quite naturally. For definiteness, I shall consider graphs with undirected links only.

When one is talking about *random graphs*, one has of course in mind a statistical ensemble of graphs. How to define such an ensemble? The simplest answer is given in the framework of the classical model developed by Erdős, Rényi and their followers [2]: in a set of N vertices one connects at random L out of $N(N-1)/2$ possible pairs of vertices. All possible graphs constructed that way form the ensemble in question. The probability p to connect a pair of vertices is the control parameter of the model. The geometry of graphs changes in a very interesting and by now fully understood manner when p changes. However, in this ensemble the distribution of connectivity (vertex degree) is always Poissonian.

It turns out that connectivity distributions very different from Poissonian are observed in a variety of observed networks. In particular, in a number of interesting networks this distribution has a tail falling like a power of the vertex degree. These networks have been baptized *scale-free* by Barabási and Albert [3]. The properties of scale-free networks are commonly discussed in the framework of simple growth models (where the connectivity distribution becomes stationary and scale-free at large time). These models are invaluable for illustrating basic dynamical mechanisms, like the preferential attachment rule. However, they are not fully realistic. For a variety of reasons one would like to understand the generic geometries of wide classes of graphs. This can be presumably better achieved by defining consistently the corresponding statistical ensembles, instead of producing more and more complicated growing network models.

The aim of this talk is to discuss problems one encounters trying to define a statistical ensemble of random graphs with an *a priori* given connectivity distribution. The definition can be more or less formal. It can be implicit, reducing to the formulation of an algorithm enabling one to sample graphs, for example with the help of a computer.

2 The Molloy-Reed construction

Let p_n denote here the connectivity distribution. In ref. [4] Molloy and Reed propose a specific method of constructing graphs with a given p_n . They proceed in two steps:

(a) First, N auxiliary graphs are created. The number of links of an auxiliary graph is randomly generated from the probability distribution p_n . By construction all these links meet at a common vertex and have the other end free. The number of free-end links in the full set of auxiliary graphs must be even, otherwise one restarts the construction.

(b) Second, in the full set of N auxiliary graphs the successive pairs of free link ends are picked at random and connected, until no free link end remains.

In this manner, one creates a single graph with vertex degrees n_1, n_2, \dots, n_N . Notice, that the number of links of that graph $L = 1/2 \sum_j n_j$ is not kept fixed. In the ensemble of graphs it does fluctuate around the average value $1/2N\langle n \rangle$, where $\langle \dots \rangle = \sum_n \dots p_n$. This is perhaps a weak point of the construction, since L/N is a sensitive parameter in graph theory. On the other hand, it is very pleasant that the connectivity distribution matches p_n for *individual graphs*.

Notice also that these graphs are, in general, not connected. Furthermore, they are, in general, "degenerate": there may be multiple connections between vertices and certain links may connect a vertex to itself¹. For a given set n_1, n_2, \dots, n_N a non-degenerate graph may simply not exist. Moreover, enforcing non-degeneracy, when it is possible, introduces a bias. Although in each graph the connectivity distribution matches p_n up to fluctuations, significant deviations from p_n can appear, when the distribution is calculated for a large ensemble of graphs, if certain fluctuations are systematically favoured. This remark is particularly pertinent to the case of scale-free graphs, where the connectivity distribution has a long tail, subject to important fluctuations.

¹I met the opinion that in this construction the degenerate graphs become unimportant in the limit $N \rightarrow \infty$. This is false. It is easy to count graphs. When $N \rightarrow \infty$ and $x = L/N$ is kept fixed, the non-degenerate graphs are a finite fraction, viz. $\exp[-2x(1+x)]$, of all possible graphs.

3 Minifield theory: random graphs and Feynman diagrams

The minifield theory is defined by the following formal integral

$$Z \sim \int d\phi \exp \frac{1}{\kappa} [-\phi^2/2\lambda + \sum_n p_n \phi^n] \quad (1)$$

where the integration variable ϕ is a real number, $\kappa, \lambda, p_1 > 0$ and $p_n \geq 0$ for $n > 1$. Although, strictly speaking, the integral does not exist, the perturbative expansion of Z in powers of the "couplings" p_n is well defined. As in field theory, the individual terms of the expansion can be represented by Feynman diagrams. The "propagator" equals λ , κ plays the role of the Planck constant and p_1 that of an "external current" (a pedagogical presentation for people not very familiar with field theory methods can be found in [1]).

The idea is to identify the Feynman diagrams of this toy model with the graphs of a statistical ensemble. Indeed, the Feynman diagrams of the minifield theory are the graphs familiar to people working on networks, except that there is a specific weight - the "Feynman amplitude" - attached to each graph. In the "semiclassical limit" $\kappa \rightarrow 0$ only tree graphs survive and the model is exactly solvable.

According to the Feynman rules, the weight of a non-degenerate graph with N vertices and L links is

$$weight = \kappa^{L-N} \frac{\lambda^L}{N!} \prod_{j=1}^N [p_{n_j} n_j!] \quad (2)$$

In the presence of degeneracies one has to multiply the rhs by the standard symmetry factors. Actually, the construction of Feynman diagrams does not differ from the construction of graphs following the Molloy-Reed recipe. Here, the auxiliary graphs are those defined by the "interactions" $p_n \phi^n$. However, the weight factor $\kappa^{L-N} \lambda^L / N!$ does not appear there; the fluctuations of L result from fluctuations of the generated vertex degrees. In contrast, we introduce here a specific fugacity of links λ and a parameter, κ , controlling the number of loops in connected components.

The following Metropolis algorithm generates graphs with fixed N and L : one picks a random link \vec{ij} and a random vertex $k \neq i, j$ and one rewires $\vec{ij} \rightarrow \vec{ik}$ with probability

$$P_{rewire} = (n_k + 1)R(n_k + 1)/n_j R(n_j) \quad (3)$$

when the rhs above is less than unity, and with probability equal to one otherwise. Here $R(n) = p_n/p_{n-1}$. When $n_j = 1$, the attempt is rejected, so that vertices with zero connectivity are never created. The rhs of (3) follows from (2) and the detailed balance condition. It turns out, that this last condition insures that the symmetry factors in the weights of degenerate graphs come out correctly too.

The presence of the factor $(n_k + 1)/n_j$ on the rhs of (3) means that the rewired vertices are sampled independently of their degree. Furthermore, the rewiring depends on the vertex degrees only and is insensitive to the rest of the underlying graph structure. Hence, as far as the distribution of vertex degrees is concerned, the model is isomorphic to the well known balls-in-boxes model [5], defined by the partition function

$$z \sim \sum_{n_j} p(n_1) \dots p(n_N) \delta(M - \sum_{j=1}^N n_j) \quad (4)$$

and describing M balls distributed with probability p_n among N boxes (in our case $M = 2L$). The constraint represented by the Kronecker delta on the rhs of (4) is satisfied "for free" when $N \rightarrow \infty$ by virtue of Khintchin's law of large numbers, provided $\langle n \rangle < \infty$ and $M/N = \langle n \rangle$. When the last condition is met the occupation number distribution of a single box is just p_n .

Consequently, in the statistical ensemble including *degenerate* graphs the connectivity distribution is p_n provided the number of links is set to $L = 1/2N\langle n \rangle$ (notice, that it is the average number of links in the Molloy-Reed construction). It is easy to calculate the number of such graphs for fixed L/N . It increases with N like $\exp[\text{const}N \log N]$, the ensemble is overextensive². Hence, it is not guaranteed that the connectivity distribution is p_n for individual graphs, it is so when one averages over the ensemble. This should not be a serious flaw in applications.

The algorithm works also very well for *trees*. It suffices to start with a tree graph, for example with a polyline, and impose the constraint that $n_i = 1$. Then, all successively generated graphs are also trees. As already mentioned, the model is analytically solvable when one limits one's attention to tree graphs. One can show exactly that in this case the connectivity distribution is $\sim np_n$ ³. Hence, in order to get an *a priori* given connectivity distribution P_n one should set the couplings of the tree model to $p_n \sim P_n/n$.

² The ensemble of non-degenerate graphs is overextensive too (cf the footnote on p. 3); it becomes extensive in the limit $\kappa \rightarrow 0$, ie for tree graphs.

³The following heuristic argument can help to understand that: trees can always be

A fairly comprehensive discussion of the ensemble of random tree graphs is presented in [1], with emphasis on the hot problem of scale-free graphs. I shall not enter into this discussion here, apart from the few words to follow. The partition function (1) can be calculated in the saddle point ("semi-classical") approximation. The saddle point condition, identical to a familiar equation in polymer physics, is a starting point for further calculations. In particular, one can find the fractal dimension d_H of the tree graphs. This was first done in [6] for the so-called generic case, with the result $d_H = 2$. For scale-free graphs the connectivity distribution falls like $n^{-\beta}$ and one finds [7, 1] in the empirically interesting situation $2 < \beta \leq 3$:

$$d_H = (\beta - 1)/(\beta - 2) \quad (5)$$

while $d_H = 2$ again for $\beta > 3$. An infinite d_H is found in the rather special case, where a singular vertex with fixed degree of order $O(N)$ is present in (almost) all trees of the ensemble ⁴.

It is very easy to supplement the algorithm with a constraint insuring that all produced graphs are non-degenerate. However, this introduces a bias. We do not know yet how to choose the input data, ie the couplings p_n , in order to get at the output a desired connectivity distribution. The problem is solved for degenerate graphs and for trees, as stated above, but for non-degenerate graphs it remains open:

Query : What are the minifield theory couplings p_n leading to a given connectivity distribution in the ensemble of *non-degenerate* graphs ?

The ensemble of graphs defined by (1) is fairly general, but not the most general one: the weight of a graph is a product of factors corresponding to individual vertices. One can introduce correlations between neighbor vertices replacing (1) by

$$Z \sim \int d^q \phi \exp \frac{1}{\kappa} [-\vec{\phi} A \vec{\phi} + \sum_{n=1}^q \phi_n^n] \quad (6)$$

where $\vec{\phi} = (\phi_1, \phi_2, \dots, \phi_q)$ and A is some $q \times q$ symmetric matrix with positive elements. The cut-off q can be eventually sent to infinity (but in order to

embedded in a plane. They are obtained by gluing successive vertices (auxiliary graphs). But each vertex with n links attached to it could have been rotated in the plane up to n times before being glued to the tree it belongs to and this rotation would not affect the result. Consequently, the weight of a vertex is $\sim np_n$ instead of p_n , because of this specific symmetry.

⁴The Cayley tree, a graph with a minimal entropy in our ensemble, also has $d_H = \infty$.

study the tree content of the model the limit $\kappa \rightarrow 0$ should be taken first). This model has not been studied yet:

Query: What are the properties of the ensemble defined by (6), for reasonable choices of the correlation inducing matrix A ? Even a study of the "semiclassical" limit alone would be of interest.

4 Growing networks

Recently, much activity has been devoted to the formulation of growing network algorithms producing the so-called scale-free graphs (see, for example, refs. [3, 8, 9]). In these models and at large "time" the average connectivity becomes stationary, except for the tail where finite size (time!) corrections are felt. A repeated use of such a growing network algorithm defines a statistical ensemble and, with this strategy, it is not difficult to produce non-degenerate graphs only. The connectivity distribution cannot be chosen at will, it has a shape specific to the model at hand. But one can usually adjust the parameters of the algorithm to control the large vertex degree behavior. The major problem with this approach is that it is difficult to decide whether the results one obtains are generic or just reflect the specific dynamics of a rather simple model.

Let me illustrate this point with an example in the next section.

5 Graph diameters

Consider *tree* graphs with connectivity distribution

$$P_n = \frac{4}{n(n+1)(n+2)} \quad (7)$$

They can be generated by the Barabasi-Albert growing network recipe [3, 8], or by the algorithm presented in Sec. 3, provided the couplings are set to $p_n = P_n/n$. For a given graph let $n(r)$ denote the number of vertices separated by geodesic distance r from a randomly chosen "reference" vertex. Averaging over the ensemble of graphs one is interested in and over the possible choices of the "reference" vertex, one gets a specific "two-point function" $\langle n(r) \rangle$, which can be used to define the average diameter of a graph. All this is easily done on a computer. The result, illustrated in Figs 1 and 2,

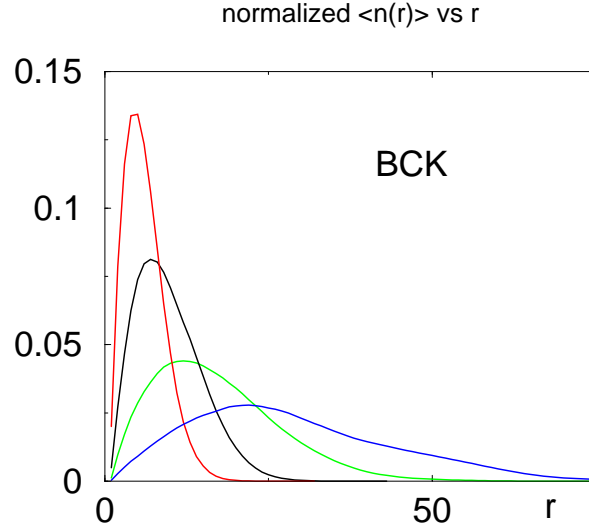


Figure 1: The normalized two-point function $\langle n(r) \rangle$ in the statistical ensemble defined in [1] calculated for the number of nodes $N = 100, 400, 1600, 6400$. The connectivity distribution is given by eq (7).

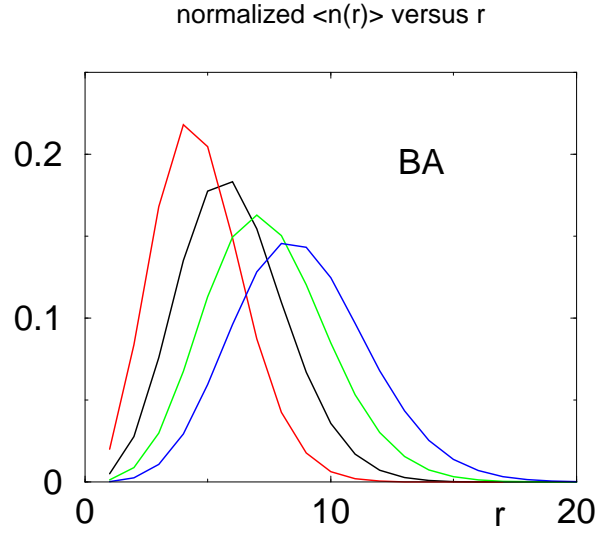


Figure 2: The normalized two-point function $\langle n(r) \rangle$ in the ensemble of graphs generated by the growing network algorithm proposed by Barabasi-Albert in [3], calculated for the number of nodes $N = 100, 400, 1600, 6400$. The connectivity distribution is given by eq (7).

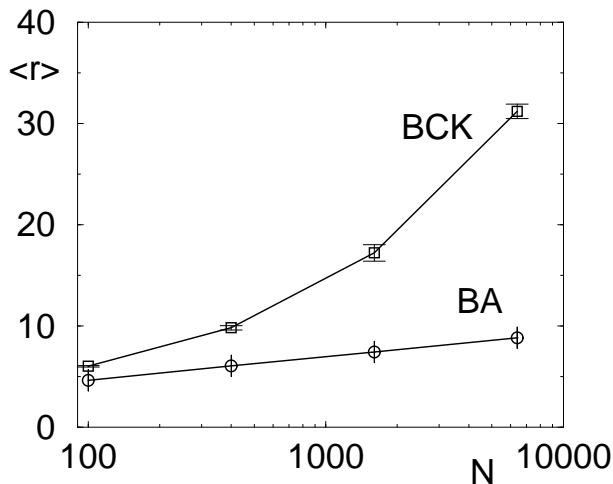


Figure 3: The average size of a graph $\langle r \rangle$ versus N in the two models. It is seen that in the Barabasi-Albert model the growth of $\langle r \rangle$ is logarithmic.

is that $\langle n(r) \rangle$ is very different in the two models. In the Barabasi-Albert model the graph diameter grows like $\log N$, while in the model of Sec. 3 it grows like a power of N (see Fig. 3). Manifestly, the Barabasi-Albert model explores only a fraction of available phase-space. This is simply explained: the vertices of highest degree are the oldest ones and tend in this model to be close to each other. Consequently, the distance between other vertices is also much smaller than in a truly random tree. Another deviation from randomness in growing networks was observed earlier by Callaway et al [10].

Incidentally, it appears that $\langle r \rangle \sim \log N$ in the ensemble of *degenerate* graphs with the same P_n generated by the algorithm of Sec. 3 (see Fig. 4). Intuitively it is obvious that the growth of the diameter becomes slower when loops can be formed often enough since they produce "shortcuts".

Actually, the "small world" behavior $\langle r \rangle \sim \log N$ is found in a large variety of networks. I do not know any rigorous derivation of this result in a sufficiently general context. In the network community one often refers to ref. [11]. Unfortunately, although ref. [11] is otherwise an interesting paper, their derivation of this logarithmic growth is mathematically incorrect. They have in mind the Molloy-Reed construction, but they actually consider tree

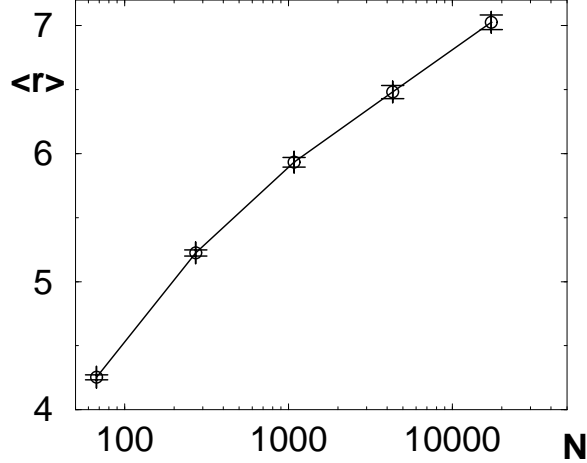


Figure 4: The average size $\langle r \rangle$ of the giant component versus N = average #nodes in the component for general (degenerate) graphs with loops. N is not very large and finite size correction to $\langle r \rangle$ is important. The connectivity distribution is (7) for the full graph and falls also roughly like $\sim n^{-3}$ for the giant component.

graphs with uncorrelated vertex degrees, and for such trees the diameter usually grows as a power of N .

To see the mistake, notice that for a given "reference" vertex one has

$$1 + n(1) + n(2) + \dots + n(r_{max}) = N \quad (8)$$

Newman et al replace all the quantities in (8) by their bulk average values. However, this is, in general, illegal. With each "reference" point is associated a specific sequence $n(1), n(2), \dots$. The conditional probability that $n(r) = k$ differs from the bulk probability that a vertex has k r^{th} -near-neighbors. It depends on the sequence leading to $n(r)$. One has to attach probability measures to possible sequences in graphs and also to graphs. The problem is not trivial but it was solved by Ambjørn et al [6] precisely for the class of connected tree graphs considered in ref. [11]. The result is that generically the Hausdorff dimension is finite and therefore the graph diameter grows like a power of N , as already mentioned. Hence, I end this talk with another query:

Query: What are the general conditions insuring that the "small world" behavior $\langle r \rangle \sim \log N$ does actually hold as an exact result for $N \rightarrow \infty$?

A nice theorem awaits for being formulated and proved!

I wish to thank Serguei Dorogovtsev for pointing out to me that an argument used in the original version of this text is spurious.

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